O 93: Scanning Probe Techniques: Method Development

Time: Thursday 15:00–18:00 Location: MA 043

O 93.1 Thu 15:00 MA 043

Tip-to-tip approach for multi-probe scanning probe microscopy utilizing long-distance all-optical methods — •Philipp Lindner, Raluca Boltje, Jonas Koch, Stefan Krause, and Roland Wiesendanger — Department of Physics, University of Hamburg, Germany

In multi-probe scanning probe microscopy, scanning electron microscopy (SEM) is conventionally used to support the individual positioning of the probes. However, SEM is incompatible with the application of high magnetic fields, eventually contaminates high-quality sample surfaces, and is limited to close working distances. Here we present the employment of a Maksutov-Cassegrain telescope (MCT) and a high-irradiance focused fiber-optic illumination system to achieve a diffraction-limited optical resolution of 3 micrometers at a working distance greater than 50 cm for three-tip spin-polarized scanning tunneling microscopy experiments at low temperatures and high magnetic fields. The oblique angle between the MCT objective lens and the sample plane, in combination with Airy pattern interference between the probe tips and their mirror images reflected from the specular sample surface, is utilized for the three-dimensional positioning of the probe tips into overlapping scan ranges. In contrast to SEM-based approaches, our method is applicable to compact scanning probe microscopes installed into the confined geometries of a superconducting magnet cryostat.

O 93.2 Thu 15:15 MA 043

Multi-Probe RF Scanning Tunneling Microscopy in UHV, at Low Temperatures, and in Magnetic Fields — •Jonas Koch, Philipp Lindner, Raluca Boltje, Stefan Krause, and Roland Wiesendanger — Department of Physics, University of Hamburg, Germany

We present a three-tip scanning tunneling microscope designed for multi-probe investigations on the atomic scale. It was developed for the operation in an ultra-high vacuum chamber system [1], at temperatures between 1.5 K and 100 K, and in an external magnetic field of up to 3 T. Three independent scanning units are capable of spin-polarized tunneling with atomic spatial and picosecond time resolution. Ultrasharp tunneling tips are brought into overlapping scan ranges. One of the potential applications is the localized generation of high-density surface current at low total currents, thereby minimizing harming effects like Joule heating. We will present first proof-of-concept experiments on the example of a local surface current application, along with respective numerical modelling of the electrical current on the sample surface. [1] J. Friedlein *et al.*, Rev. Sci. Instrum. **90**, 123705 (2019).

O 93.3 Thu 15:30 MA 043

Spin-Polarized Transport at the Atomic Limit — •Markus Leisegang, Patrick Härtl, Jens Kügel, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Transport measurements that are sensitive to the band structure of a material require techniques that operate on the length scale of the charge carrier's mean free path. In order to get real space access to charge carrier transport at distances of the mean free path and thus in the ballistic regime, we developed and established the molecular nanoprobe (MONA) technique [1,2].

Hereby, we use a single molecule as a detector for charge carriers, which are injected into the substrate under investigation by the STM tip a few nanometers away from the molecule. The high spatial resolution of MONA combined with the small size of the molecular detector allows for transport paths which can be controlled at the atomic level. In a very recent experiment, we merged the MONA technique with spin-polarized STM to SP-MONA. By using the Rashba-split surface state of the $BiAg_2$ surface as a test sample, we proof that this technique allows to detect spin-polarized transport at the atomic limit [3].

[1] J. Kügel *et al.*, Nano Lett. **17**, 5106 (2017)
[2] M. Leisegang *et al.*, Nano Lett. **18**, 2165–2171 (2018)
[3] P. Härtl *et al.*, arXiv:2303.00393 (2023)

O 93.4 Thu 15:45 MA 043

Autonomous chemical reactions in scanning tunneling microscope — •Nian Wu[1], Markus Aapro[1], Alexander Ilin[2], Robert Drost[1], Joakim Jestilä[1], Zhijie He[2], Peter Liljeroth[1], and Adam S. Foster[1,3] — [1]Applied Physics, Aalto University, Espoo, Finland — [2]Computer Science, Aalto University, Espoo, Finland — [3]WPI Nano Life Science Institute, Kanazawa University, Kanazawa, Japan

Several breakthrough studies have harnessed scanning probe microscopy (SPM) manipulations to control chemical reactions in on-surface molecular synthesis. In general, for scanning tunnelling microscope (STM) manipulations, they are predominantly controlled via parameters of the tip position, pulse voltages and tunneling conductance. However, the selection of proper parameters requires extensive domain knowledge, which is time consuming and not necessarily transferable to new systems. Recent research has allowed the automation of a wide range of challenges in SPM, including image quality assessment, lateral and vertical manipulation. However, the automation for breaking or forming covalent bonds, which is an indispensable step during chemical synthesis is, as yet, unexplored. To address this problem, we build on our deep reinforcement learning approach to automate bromine removal from 5,15-bis(4-bromo-2,6-methyl-phenyl)porphyrin (Br2Me4DPP) through learning manipulation parameters in STM. We further explore the potential of automated STM to then controllably react the resultant fragments into larger molecular structures.

O 93.5 Thu 16:00 MA 043

Single crystal diamond needles as sensor in scanning probe microscopy — •Stefan Schulte[1,2], Sven Just[1,3], Victor I. Kleshch[4], F. Stefan Tautz[1,3], and Ruslan Temirov[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Cologne, Germany — [3]Fundamentals of Future Information Technology, Jülich Aachen Research Alliance (JARA), Jülich, Germany — [4]Moscow, Russia

It was recently demonstrated that an SPM tip carrying a quantum dot allows for the measurement of electrostatic surface potentials, in technique that is referred to as scanning quantum dot microscopy (SQDM) (Wagner et al., Phys. Rev. Lett., 2015). Here, we report on an attempt to fabricate a SQDM tip with a CVD-grown single crystal diamond needle (Kleshch et al., Phys. Rev. B, 2020; Kleshch et al., Carbon, 2021). Using the micro-manipulator inside a focussed ion beam microscope the diamond needle is attached to a needle sensor. The diamond tip needle sensor is then characterized by performing non-contact AFM and field emission experiments at room temperature UHV conditions. At elevated field emission currents of several hundred nanoamperes, a surface conductive layer forms on the diamond needle, that eventually allows us to observe electron tunneling between the tip and the surface.

O 93.6 Thu 16:15 MA 043

Systematic protocol to prepare SPM tips for Scanning Quantum Dot Microscopy — •Tim Dierker, Paul Laubrock, and Philipp Rahe — Universität Osnabrück

Scanning probe microscopy (SPM) is an established family of techniques for high-resolution measurements of surfaces. One of its variants is scanning quantum dot microscopy (SQDM) [1], a technique that enables the quantitative mapping of the electrostatic potential at the atomic scale [2]. Central for SQDM is the controlled functionalization of the SPM tip with a single molecule that acts as a quantum dot. In this work we perform low-temperature manipulation experiments with 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) molecules on Ag(111) with a combined scanning tunneling and atomic force microscope system. From the classification of manipulation and pick-up data we develop a routine to isolate single molecules from the edges of PTCDA islands and to attach them to the tip. The experimental observations allow to condense the physical complexity of the tip-molecule system into an instructive flowchart for an efficient preparation of SQDM tips.

[1] C. Wagner et al., PRL 115, 026101 (2015)
[2] C. Wagner et al., Nat. Mater. 18, 853 (2019)

O 93.7 Thu 16:30 MA 043

Van der Waals scanning probe tips — •Abhisek Kole[1,2,4], Tobias Wichmann[1,2,4], Keda Jin[1,2,3], Jia Grace Lu[5], Xiaosheng Yang[6,7], F. Stefan Tautz[1,2,4], Markus Ternes[1,2,3], Jose Martinez Castro[1,2,3], and Felix Lüpke[1,2] — [1]Peter Grünberg Institut

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Van der Waals materials are known for their intriguing emergent 2D physics, such as correlated phenomena and topological effects. Here, we report the methodical fabrication of van der Waals scanning tunnelling tips from exfoliated graphite flakes with a graphene-like edge as a scanning tunnelling tip. The principle of STM is based on the quantum mechanical tunneling between the tip and sample, revealing the convoluted underlying electronic structure. We characterize the tip by performing atomically resolved STM of an Ag(111) surface. The tip-sample differential conductance dI/dV reveals direct evidence of tunnelling through a graphene nanoribbon-like zigzag edge state, which we support by tight binding calculations.

O 93.8 Thu 16:45 MA 043

A versatile Peak Force IR variation for correlative nanoscale chemical and mechanical AFM-IR — •Martin Wagner, Qichi Hu, Chunzeng Li, Shuiqing Hu, Chanmin Su, and Peter Dewolf — Bruker Nano Surfaces, Santa Barbara CA 93117, USA

Nanoscale infrared (nano-IR) microscopy enables label-free chemical imaging and spectroscopy at the nanometer scale by combining atomic force microscopy (AFM) with infrared radiation. Over the last years, AFM-IR has been developed with different AFM modes: the original photothermal induced resonance enhanced mode and the recently developed surface sensitive technique are based on contact mode, while Tapping AFM-IR is built on tapping mode [1]. Peak Force Tapping based Peak Force infrared (PFIR) microscopy [2] has lately joined as another AFM-IR mode. All these nano-IR variations inherit the advantages and limitations of their respective AFM base mode. In this work, we focus on the capabilities offered by a PFIR-related approach, and illustrate those with examples on a variety of polymer samples. We discuss (1) the capability to perform simultaneous multimodal imaging collecting both mechanical properties such as elastic modulus together with chemical information, (2) methods to understand and decouple artifacts induced by variations in mechanical properties from the AFM-IR data, and (3) the combination with other AFM-IR techniques such as the surface sensitive mode while, at the same time, minimizing lateral forces to allow one to study soft & fragile samples.

[1] J. Mathurin et al., J. Appl. Phys. 131, 010901 (2022).
[2] L. Wang et al., Chem. Soc. Rev. 51, 5268 (2022).

O 93.9 Thu 17:00 MA 043

Approaching unstable periodic states in dynamic Atomic Force Microscopy — •Lukas Böttcher[1], Hannes Wallner[2], Niklas Kruse[2], Anna Dittus[2], Wolfram Just[2], Ingo Barke[1], Jens Starke[2], and Sylvia Speller[1] — [1]Institute of Physics, University of Rostock — [2]Institute of Mathematics, University of Rostock

Bistable states, caused by the nonlinear tip-sample interaction, are frequently encountered during dynamic Atomic Force Microscopy (AFM) measurements, sometimes leading to characteristic image artifacts. These states are characterized by two stable states, one at low, one at high amplitude, flanking an unstable branch at intermediate amplitudes. This unstable branch is usually not accessible experimentally. Utilizing fast, minimally invasive control schemes we were able to approach such states of instability. The aim is to reveal the whole resonance curve of our cantilever including fold bifurcation points and a cusp, while interacting with the surface. This may bring new insights into AFM as well as in the tip-sample contact.

O 93.10 Thu 17:15 MA 043

Total variation denoising for microscopy images — •Marco Corrias[1,2], Thomas Pock[4], and Cesare Franchini[1,3] — [1]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Vienna, Austria — [2]University of Vienna, Vienna Doctoral School in Physics, Vienna, Austria — [3]University of Bologna, Department of Physics and Astronomy, Bologna, Italy — [4]Institute of Computer Graphics and Vision, Graz University of Technology, Graz, Austria

Experimentally acquired images are affected by the ubiquitous presence of noise, which degrades their quality and hides their features. With the increase of image acquisition rate in recent years, modern denoising solutions have become necessary. This study focuses on microscopy image denoising, specifically those obtained through atomic force microscopy (AFM), scanning tunneling microscopy (STM), scanning electron microscopy (SEM), and scanning transmission electron microscopy (STEM). A total variation (TV)-based workflow is presented to automatically denoise microscopy images with different types of noise, proving that the Huber-ROF and TGV-L1 are effective to accomplish this task. Our results suggest a wider applicability of this method in microscopy, not only restricted to STM, AFM, SEM, and STEM images. The Python code used for this study will be made publicly available as part of the AiSurf package. It is designed to be integrated into experimental workflows for image acquisition or can be used to denoise previously acquired images.

O 93.11 Thu 17:30 MA 043

Image interpretation methods for high-resolution SPM — •Lauri Kurki[1], Niko Oinonen[1,2], and Adam S. Foster[1,3] — [1]Aalto University, Finland — [2]Nanolayers Research Computing Ltd., UK — [3]WPI-NanoLSI, Kanazawa University, Japan

Scanning tunnelling microscopy (STM) and atomic force microscopy (AFM) functionalized with a CO molecule on the probe apex capture sub-molecular level detail of the electronic and physical structures of a sample from different prespectives [1]. However, the produced images are often difficult to interpret. To accelerate the analysis, we propose automated machine learning image interpretation tools to extract sample properties directly from SPM images.

In recent years, there has been rapid development in image analysis methods using machine learning, with particular impact in medical imaging. These concepts have been proven effective also in SPM in general and in particular for extracting sample properties from AFM images [2,3,4]. We build upon these models and show that we can extract atomic positions directly from STM images. We also further explore how the accuracy of these predictions varies with the use of a simultaneous AFM signal. Finally, we establish the limits of the approach in an experimental context by predicting atomic structures from STM images of 2D ice structures.

[1] Cai et al. J. Am. Chem. Soc. 2022, 144, 44, 20227-20231 [2] Alldritt et al., Sci. Adv. 2020; 6 : eaay6913 [3] Carracedo-Cosme et al., Nanomaterials 2021, 11, 1658. [4] Oinonen et al., MRS Bulletin 2022, 47, 895-905

O 93.12 Thu 17:45 MA 043

Automated prediction of three-dimensional molecular structures from Atomic Force Microscopy images — •Joakim S. Jestilä[1], Shuning Cai[1], Niko Oinonen[1], Peter Liljeroth[1], and Adam S. Foster[1,2] — [1]Department of Applied Physics, Aalto University, 00076 Aalto, Espoo, Finland — [2]Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kanazawa 920-1192, Japan

Identification of three-dimensional features in surface-adsorbed molecules imaged by Atomic Force Microscopy (AFM) represents a great challenge. While the structures of planar molecules can often be recognised by human users, deviation from planarity contributes to images that are non-intuitive and difficult to interpret, even for experts. Fortunately, neural networks are well-suited for extracting the embedded information in such images. Still, the latter cannot directly determine the placement of atoms that do not contribute to the image contrast, such as atoms eclipsed by those closest to the AFM-tip. In an attempt to access the hidden atoms in the lower layers, we supplement the prediction of the upper atoms with an algorithm that provides candidate structures based on their physical feasibility, evaluated hierarchically in terms of chemical connectivity and the corresponding density functional theory energy. We demonstrate the applicability of the method in a case study of a model system for surface-adsorbed lignocellulosic molecules: 4-nitrophenyl-α/β-D-galacturonide on Au(111).